3,4-Dimethoxyphenylethylamine, N,N-di(acetyl)-

Inchi: InChI=1S/C14H19NO4/c1-10(16)15(11(2)17)8-7-12-5-6-13(18-3)14(9-12)19-4/h5-6,9H,7-

InchiKey: DCSJIDRSSJQJSD-UHFFFAOYSA-N

Formula: C14H19NO4

SMILES: COc1ccc(CCN(C(C)=O)C(C)=O)cc1OC

Mol. weight [g/mol]: 265.31

Physical Properties

Property code	Value	Unit	Source
gf	-196.91	kJ/mol	Joback Method
hf	-540.77	kJ/mol	Joback Method
hfus	33.87	kJ/mol	Joback Method
hvap	70.71	kJ/mol	Joback Method
log10ws	-2.31		Crippen Method
logp	1.641		Crippen Method
mcvol	209.220	ml/mol	McGowan Method
pc	2121.68	kPa	Joback Method
rinpol	2072.00		NIST Webbook
rinpol	2072.00		NIST Webbook
tb	721.38	K	Joback Method
tc	925.97	K	Joback Method
tf	475.79	K	Joback Method
vc	0.777	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	578.47	J/mol×K	721.38	Joback Method
cpg	592.90	J/mol×K	755.48	Joback Method
cpg	606.42	J/mol×K	789.58	Joback Method
cpg	619.03	J/mol×K	823.67	Joback Method
cpg	630.73	J/mol×K	857.77	Joback Method
cpg	641.55	J/mol×K	891.87	Joback Method
cpg	651.48	J/mol×K	925.97	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U374298&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume